

Filter Pattern Search Algorithms for Mixed Variable Constrained Optimization Problems

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Abstract: A new class of algorithms for solving nonlinearly constrained mixed variable optimization problems is presented. This class combines and extends the Audet-Dennis Generalized Pattern Search (GPS) algorithms for bound constrained mixed variable optimization, and their GPS-filter algorithms for general nonlinear constraints. In generalizing existing algorithms, new theoretical convergence results are presented that reduce seamlessly to existing results for more specific classes of problems. While no local continuity or smoothness assumptions are required to apply the algorithm, a hierarchy of theoretical convergence results based on the Clarke calculus is given, in which local smoothness dictate what can be proved about certain limit points generated by the algorithm. To demonstrate the usefulness of the algorithm, the algorithm is applied to the design of a load-bearing thermal insulation system. We believe this is the first algorithm with provable convergence results to directly target this class of problems.

1 Introduction

We introduce a new class of derivative-free filter algorithms for mixed variable optimization problems with general nonlinear constraints. Mixed variable optimization problems [6] are characterized by a mixture of continuous and categorical variables, the latter being discrete variables that must take on values from a predefined list or set of categories, or else the problem functions cannot be evaluated. Thus, continuous relaxations are not possible. These variables may be, and often are, assigned numerical value, but these values are typically meaningless. Type of material, color, and shape are common examples.

In formulating the mixed variable programming (MVP) problem, we note that changes in the discrete variables can mean a change in the constraints, and even a change in problem dimension. Thus, we denote n^c and n^d as the *maximum* dimensions of the continuous and discrete variables, respectively, and we partition each point $x = (x^c, x^d)$ into continuous variables $x^c \in \mathbb{R}^{n^c}$ and discrete variables $x^d \in \mathbb{Z}^{n^d}$. We adopt the convention of ignoring unused variables.

The problem under consideration, can be expressed as follows:

$$\begin{aligned} \min_{x \in X} \quad & f(x) \\ \text{s.t.} \quad & C(x) \leq 0, \end{aligned}$$

where $f : X \rightarrow \mathbb{R} \cup \{\infty\}$, and $C : X \rightarrow (\mathbb{R} \cup \{\infty\})^p$ with $C = (C_1, C_2, \dots, C_p)^T$. The domain $X = X^c \times X^d$ is partitioned into continuous and discrete variable spaces $X^c \subseteq \mathbb{R}^{n^c}$ and $X^d \subseteq \mathbb{Z}^{n^d}$, respectively, where X^c is defined by a finite set of bound and linear constraints,

dependent on the values of x^d . That is,

$$X^c(x^d) = \{x^c \in \mathbb{R}^{n^c} : \ell(x^d) \leq A(x^d)x^c \leq u(x^d)\},$$

where $A(x^d) \in \mathbb{R}^{m^c \times n^c}$ is a real matrix, $\ell(x^d), u(x^d) \in (\mathbb{R} \cup \{\pm\infty\})^{n^c}$, and $\ell(x^d) \leq u(x^d)$ for all values of x^d . Note that this formulation is indeed a generalization of the standard NLP problem, in that, if $n^d = 0$, then the problem reduces to a standard NLP problem, in which ℓ , A , and u (and hence, $X = X^c$) do not change.

The class of optimization algorithms discussed in this paper treats X by the “barrier” approach. Rather than applying the algorithm to f , it is applied to $f_X \equiv f + \psi_X$, where ψ_X is the indicator function of X , which takes on a value of zero in X and $+\infty$ elsewhere. This will not affect the convergence results, since these results will depend on the smoothness of f , not f_X .

Torczon [28] introduced the class of generalized pattern search (GPS) methods for solving unconstrained NLP problems, unifying a wide variety of existing derivative-free methods, and proving convergence of a subsequence of iterates to a stationary point, under the assumptions that all iterates lie in a compact set and that the objective function f is continuously differentiable in a neighborhood of the level set $\mathcal{L}(x_0) = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$ defined by the initial point $x_0 \in \mathbb{R}^n$. Under similar assumptions, Lewis and Torczon extended pattern search to bound [22] and linearly constrained problems [23] by ensuring that directions used in the algorithm include tangent cone generators of all nearby constraints, thereby ensuring convergence of a subsequence of iterates to a Karush-Kuhn-Tucker (KKT) point. Lewis and Torczon [21] also establish the connection between pattern search methods and the positive basis theory of Davis [14], in which they generalize [28] to allow the use of any set of directions that positively span \mathbb{R}^n , which can significantly reduce the number of function evaluations.

Audet and Dennis [6] extended pattern search to bound constrained MVP problems under the assumption of continuous differentiability of the objective function on the neighborhood of a level set in which all iterates lie. The success of the method is demonstrated in [20] on a problem in the design of thermal insulation systems, an expanded version of which is discussed and numerically solved in [2]. A further extension to linearly constrained MVP problems with a stochastic objective function is given in [27].

A more general derivative-free framework for solving linearly constrained mixed variable problems is introduced in [26]. Instead of applying pattern search to the continuous variables, mathematical conditions are established, by which a suitably chosen derivative-free method could be used as a local continuous search and ensure convergence to a first-order KKT point. A general derivative-based approach for large-scale unconstrained MVP problems that exploits these conditions is given in [25].

An equivalent formulation of GPS for linearly constrained NLP problems was introduced and analyzed by Audet and Dennis [7] for functions that are less well-behaved. They apply the nonsmooth calculus of Clarke [12] to establish convergence properties for functions lacking

the smoothness properties of those studied in previous work. In doing so, they present a hierarchy of convergence results for bound and linearly constrained problems, in which the strength of the results depends on local continuity and smoothness conditions of the objective function. As a consequence, they establish some of the earlier results of [28], [22], and [23] as corollary to theirs.

For NLP problems with general nonlinear constraints, Lewis and Torczon [24] apply bound constrained pattern search to an augmented Lagrangian function [13] and show that, under the same assumptions as in [13], plus a mild restriction on search directions, the algorithm converges to a KKT first-order stationary point.

Audet and Dennis [8] adapt a filter method within the GPS framework to handle general nonlinear constraints. Originally introduced by Fletcher and Leyffer [15] to conveniently globalize sequential quadratic programming (SQP) and sequential linear programming (SLP), filter methods accept steps if either the objective function or an aggregate constraint violation function is reduced. Fletcher, Leyffer, and Toint [16] show convergence of the SLP-based approach to a limit point satisfying Fritz John [19] optimality conditions; they show convergence of the SQP approach to a KKT point [17], provided a constraint qualification is satisfied. However, in both cases, more than a simple decrease in the function values is required for convergence with these properties.

Audet and Dennis show convergence to limit points having almost the same characterization as in [7], but with only a simple decrease in the objective or constraint violation function required. While they are unable to show convergence to a point satisfying KKT optimality conditions (and, in fact, have counterexamples [8]), in that $-\nabla f(\hat{x})$ does not necessarily belong to the normal cone at \hat{x} , they are able to show that $-\nabla f(\hat{x})$ belongs to the polar of a cone defined by directions that are used infinitely often. Thus, a richer set of directions, although more costly, will increase the likelihood of achieving convergence to a KKT point.

The present paper introduces a filter GPS algorithm for MVP problems with general nonlinear constraints. In doing so, we rely on the nonsmooth Clarke [12] calculus as in [7] and [8] to establish a unifying hierarchy of results for all the pattern search methods to date.

The paper is outlined as follows. After presenting some basic ideas on mixed variables in Section 2, we construct the mixed variable GPS (MVPS) method of Audet and Dennis [6] in Section 3, retailored for linearly constrained MVP problems. In Section 4, we extend this development to general constraints by the use of a filter and present the Filter-MVPS algorithm. We establish the theoretical convergence properties for the new algorithm in Section 5. In Section 6, the algorithm is applied to the design of a load-bearing thermal insulation system, and some limited numerical results from [2] are provided to illustrate the usefulness of the algorithm.

2 Local Optimality for Mixed Variables

In order to solve problems with categorical variables, a notion of local optimality is needed. For continuous variables, this is well-defined in terms of local neighborhoods. However, for categorical variables, a local neighborhood must be defined by the user, and there may be no obvious choice for doing so; special knowledge of the underlying engineering process or physical problem may be the only guide.

To keep the definition as general as possible, we define local neighborhoods in terms of a set-valued function $\mathcal{N} : X \rightarrow 2^X$, where 2^X denotes the power set (or set of all possible subsets of X). By convention, we assume that for all $x \in X$, the set $\mathcal{N}(x)$ is finite, and $x \in \mathcal{N}(x)$.

As an example, one common choice of neighborhood function for integer variables is the one defined by $\mathcal{N}(x) = \{y \in X^d : \|y - x\|_1 \leq 1\}$. However, categorical variables may have no inherent ordering, which would make this choice inapplicable.

We now extend the classical definition of local optimality to mixed variable domains, by the following slight modification of a similar definition by Audet and Dennis [6].

Definition 2.1 *A point $x = (x^c, x^d) \in X$ is said to be a local minimizer of f with respect to the set of neighbors $\mathcal{N}(x) \subset X$ if there exists an $\epsilon > 0$ such that $f(x) \leq f(v)$ for all v in the set*

$$X \cap \bigcup_{y \in \mathcal{N}(x)} (B(y^c, \epsilon) \times y^d). \quad (1)$$

In order to develop and analyze algorithms for solving optimization problems over a mixed variable domain, we require a definition of a limit, and a notion of continuity for \mathcal{N} .

Definition 2.2 *Let $X \subseteq (\mathbb{R}^{n^c} \times \mathbb{Z}^{n^d})$ be a mixed variable domain. A sequence $\{x_i\} \subset X$ is said to converge to $x \in X$ if, for every $\epsilon > 0$, there exists a positive integer N such that $x_i^d = x^d$ and $\|x_i^c - x^c\| < \epsilon$ for all $i > N$. The point x is said to be the limit point of the sequence $\{x_i\}$.*

Definition 2.3 *Let $\|\cdot\|$ be any vector norm on \mathbb{R}^{n^c} . The set-valued function $\mathcal{N} : X \subseteq (\mathbb{R}^{n^c} \times \mathbb{Z}^{n^d}) \rightarrow 2^X$ is said to be continuous at $x \in X$ if, for every $\epsilon > 0$, there exists $\delta > 0$ such that, whenever $u \in X$ satisfies $u^d = x^d$ and $\|u^c - x^c\| < \delta$, the following two conditions hold:*

1. If $y \in \mathcal{N}(x)$, then there exists $v \in \mathcal{N}(u)$ satisfying $v^d = y^d$ and $\|v^c - y^c\| < \epsilon$,
2. If $v \in \mathcal{N}(u)$, then there exists $y \in \mathcal{N}(x)$ satisfying $y^d = v^d$ and $\|y^c - v^c\| < \epsilon$.

Definition 2.3 will ensure that, in the convergence theory that appears in Section 5, for certain subsequences of iterates, the limit point of a corresponding subsequence of discrete neighbor points is itself the discrete neighbor of the limit point of the subsequence of iterates.

3 Pattern Search for Linearly Constrained MVPs

In order to introduce the Filter-MVPS algorithm, it is helpful to first build up the structure by describing the GPS algorithm for linearly constrained MVP problems. Most of the discussion in this section comes from [6], but some improvements are added here, including a slightly more general mesh construction and the treatment of linear constraints and functions that are not necessarily continuously differentiable.

A pattern search algorithm is characterized by a sequence of iterates $\{x_k\}$ in X with nonincreasing objective function values. Each iteration is characterized by two key steps – an optional global SEARCH step and a local POLL step – in which the objective function is evaluated at a finite number of points (called trial points) lying on a carefully constructed mesh (to be formally defined for MVP problems later) in an attempt to find a new iterate with a lower objective function value than the current iterate (called the incumbent).

A key practical point in the Audet-Dennis GPS algorithms is that they explicitly separate out a SEARCH step from the POLL step within the iteration. In the SEARCH step, any strategy may be used in selecting a finite number of trial points, as long as the points lie on the mesh. This flexibility lends itself quite easily to hybrid algorithms and enables the user to apply specialized knowledge of the problem. The user can apply a favorite heuristic, such as random sampling, simulated annealing, a few generations of a genetic algorithm, etc., or perhaps optimize an inexpensive surrogate function on the mesh, as is common in difficult engineering design problems with expensive function evaluations [5, 10, 9, 11]. While the SEARCH step contributes nothing to the convergence theory of GPS (and in fact, an unsuitable SEARCH may impede performance), the use of surrogates enables the user to potentially gain significant improvement early on in the iteration process at much lower cost.

If the SEARCH step fails to find an *improved mesh point* (*i.e.*, a point with lower objective function value), then the POLL step is invoked, in which the function is evaluated at a set neighboring mesh points around the incumbent, called the *poll set*. The POLL step is more carefully structured, so as to help ensure the algorithm's theoretical convergence properties. If either the SEARCH or POLL step finds an improved mesh point, then it becomes the incumbent, and the mesh is retained or coarsened. If no improved mesh point is found, then x_k is said to be a *mesh local optimizer*, and the current mesh is refined.

3.1 Construction of the Mesh and Poll Set

The following construction is slightly more general than in [6]. For each combination $i = 1, 2, \dots, i_{\max}$, of values that the discrete variables may possibly take, a set of positive spanning directions D^i is constructed by forming the product

$$D^i = G_i Z_i, \quad (2)$$

where $G_i \in \mathbb{R}^{n^c \times n^c}$ is a nonsingular generating matrix, and $Z_i \in \mathbb{Z}^{n^c \times |D^i|}$. We will sometimes use $D(x)$ in place of D^i to indicate that the set of directions is associated with the discrete variable values of $x \in X$. The set D is then defined by $D = \bigcup_{i=1}^{i_{\max}} D^i$.

The mesh M_k is formed as the direct product of X^d with the union of a finite number of lattices in X^c . Each of these lattices is the union of lattices centered at the continuous part of the variables at previously visited trial points. More precisely :

$$\begin{aligned} M_k &= X^d \times \bigcup_{i=1}^{i_{\max}} M_k^i \\ \text{with } M_k^i &= \bigcup_{x \in S_k} \{x^c + \Delta_k D^i z : z \in \mathcal{Z}_+^{|D^i|}\} \subset X^c, \end{aligned} \quad (3)$$

and where $\Delta_k > 0$ is the mesh size parameter, and S_k is the set of trial points where the objective function and constraints were evaluated by the start of iteration k . We should note that the mesh is purely conceptual and is never explicitly created. Instead, directions are only generated when necessary in the algorithm.

Using this construction, we also require that the neighborhood function \mathcal{N} be constructed so that all discrete neighbors of the current iterate lie on the current mesh; *i.e.*, $\mathcal{N}(x_k) \subseteq M_k$ for all $k = 0, 1, \dots$. This will be explicitly stated as an assumption in Section 5. Also observe the each lattice in (4) is expressed as a translation from x_k^c , as opposed to y_k^c , for some $y_k \in \mathcal{N}(x_k)$. This is necessary to ensure convergence of the algorithm. This does not mean that a point and its discrete neighbors have the same continuous variable values. In fact, Kokkolaras *et al.* [20] construct their neighbor sets in a way that neighbors often do *not* have the same continuous variable values.

Polling in the MVPS algorithm is performed with respect to the continuous variables, the discrete neighbor points, and the set of points generated by an EXTENDED POLL step. At iteration k , let $D_k(x) \subseteq D^{i_0} \subset D$ denote the set of poll directions for some $x \in S_k$ corresponding to the i_0 -th set of discrete variable values. The *poll set* centered at x is defined as

$$P_k(x) = \{x\} \cup \{x + \Delta_k(d, 0) \in X : d \in D_k(x)\} \subset M_k \subset X. \quad (4)$$

We remind the reader that the notation $(d, 0)$ is consistent with the partitioning into continuous and discrete variables, respectively, where 0 means that discrete variables do not change value. Thus, $x + \Delta_k(d, 0) = (x^c + \Delta_k d, x_k^d)$.

In some cases where the poll set and set of discrete neighbors fail to produce a lower objective function value, MVPS performs an EXTENDED POLL step, in which additional polling is performed around any promising points in the set of discrete neighbors whose objective function value is sufficiently close to the incumbent value. That is, if $y \in \mathcal{N}(x_k)$ satisfies $f(x_k) \leq f(y) < f(x_k) + \xi_k$ for some user-specified tolerance value $\xi_k \geq \xi$ (called the *extended poll trigger*), where ξ is a fixed positive scalar, then we begin a polling sequence

$\{y_k^j\}_{j=1}^{J_k}$ with respect to the continuous neighbors of y_k beginning with $y_k^0 = y_k$ and ending when either $f(y_k^{J_k} + \Delta_k(d, 0)) < f(x_k)$ for some $d \in D_k(y_k^{J_k})$, or when $f(x_k) \leq f(y_k^{J_k} + \Delta_k(d, 0))$ for all $d \in D_k(y_k^{J_k})$. For this discussion, we let $z_k = y_k^{J_k}$, the last iterate (or *endpoint*) of the EXTENDED POLL step. We should note that in practice, the parameter ξ_k is typically set as a percentage of the objective function value (but bounded away from zero), such as, say, $\xi_k = \max\{\xi, 0.05|f(x_k)|\}$. A relatively high choice of ξ_k will generate more EXTENDED POLL steps, which is likely to lead to a better local solution, but at a cost of more function evaluations. On the other hand, a lower value of ξ_k will require fewer function evaluations, but it will probably result in a poorer quality local solution.

The set of extended poll points for a discrete neighbor $y \in \mathcal{N}(x_k)$, denoted $\mathcal{E}(y)$, contains a subset of the points $\{P_k(y_k^j)\}_{j=1}^{J_k}$. At iteration k , the set of points evaluated in the EXTENDED POLL step (or *extended poll set*) is given by

$$\mathcal{X}_k(\xi_k) = \bigcup_{y \in \mathcal{N}_k^\xi} \mathcal{E}(y), \quad (5)$$

where $\mathcal{N}_k^\xi = \{y \in \mathcal{N}(x_k) : f(x_k) \leq f(y) \leq f(x_k) + \xi_k\}$.

3.2 Update Rules

If either the SEARCH, POLL, or EXTENDED POLL step is successful at finding an improved mesh point, then it becomes the new incumbent x_{k+1} , and the mesh is coarsened according to the rule,

$$\Delta_{k+1} = \tau^{m_k^+} \Delta_k, \quad (6)$$

where $\tau > 1$ is rational and fixed over all iterations, and the integer m_k^+ satisfies $0 \leq m_k^+ \leq m_{\max}$ for some fixed integer $m_{\max} \geq 0$. Coarsening of the mesh does not prevent convergence of the algorithm, and may make it faster. Note that only a simple decrease in the objective function value is required.

If the SEARCH and POLL steps both fail to find an improved mesh point, then the incumbent is a mesh local optimizer and remains unchanged (or, alternatively, can be chosen as a point having the same function value as the incumbent, if one exists), while the mesh is refined according to the rule,

$$\Delta_{k+1} = \tau^{m_k^-} \Delta_k, \quad (7)$$

where $\tau > 1$ is defined above, $\tau^{m_k^-} \in (0, 1)$, and the integer m_k^- satisfies $m_{\min} \leq m_k^- \leq -1$ for some fixed integer m_{\min} .

It follows that, for any integer $k \geq 0$, there exists an integer r_k such that

$$\Delta_k = \tau^{r_k} \Delta_0. \quad (8)$$

3.3 Linear Constraints

In order to treat linear constraints and still ensure appropriate convergence results, the only requirement is that the directions that define the mesh be sufficiently rich to ensure that polling directions can be chosen that conform to the geometry of the constraint boundaries, and that these directions be used in infinitely many iterations. For our analysis, we need the following definition (from [7]), which abstracts this notion of conformity. We appeal to the construction of Lewis and Torczon [23], who provide an algorithm for choosing conforming directions using standard linear algebra tools.

Definition 3.1 *A rule for selecting the positive spanning sets $D_k(x) \subseteq D$ conforms to X at x for some $\epsilon > 0$, if at each iteration k and for each y in the boundary of X for which $\|y - x\| < \epsilon$, the tangent cone $T_X(y)$ is generated by nonnegative linear combinations of a subset of the columns of $D_k(x)$.*

Nonlinear constraints pose a problem for GPS algorithms in that choosing enough directions to conform to the geometry of the constraints (to guarantee convergence to a KKT point) would require an infinite number of directions in D , which the convergence theory does not support. Thus, a different strategy must be employed to handle nonlinear constraints. In the next section, we add a filter to do this.

4 The Filter-MVPS Algorithm

In filter algorithms, the goal is to minimize two functions, the objective f and a continuous aggregate constraint violation function h that satisfies $h(x) \geq 0$ with $h(x) = 0$ if and only if x is feasible. The function h is often set to $h(x) = \|C(x)_+\|$, where $\|\cdot\|$ is a vector norm and $C(x)_+$ is the vector of constraint violations at x ; i.e., for $i = 1, 2, \dots, m$, $C_i(x)_+ = C_i(x)$ if $C_i(x) > 0$; otherwise, $C_i(x)_+ = 0$. If the squared 2-norm is used, then h inherits whatever smoothness properties C possesses [8].

In our case, and consistent with [8], we define a second constraint violation function $h_X = h + \psi_X$, where ψ_X is the indicator function for X . It is 0 on X and $+\infty$ elsewhere. We will see in Section 5 that convergence results will depend on the smoothness of h and not h_X .

The Filter-MVPS algorithm can be viewed as either an extension of the Filter-GPS algorithm [8] for mixed variables, or as an extension of the mixed variable GPS algorithm of Audet and Dennis [6] for general nonlinear constraints. We present it here as the latter, and appeal to [8] for the construction of the filter.

4.1 Filters

The definition of dominance provided below, which comes from the multi-criteria optimization literature, is adapted from a similar term in [15], so that it is defined with respect to the objective function f and constraint violation function h . This adaptation is consistent with [8]. A formal definition of a filter follows immediately thereafter.

Definition 4.1 *A point $x \in \mathbb{R}^n$ is said to dominate $y \in \mathbb{R}^n$, written $x \prec y$, if $f(x) \leq f(y)$ and $h_X(x) \leq h_X(y)$ with either $f(x) < f(y)$ or $h_X(x) < h_X(y)$*

Definition 4.2 *A filter, denoted \mathcal{F} , is a finite set of points in the domain of f and h such that no pair of points x and y in the set have the relation $x \prec y$.*

In constructing a filter for GPS algorithms, we put two additional restrictions on \mathcal{F} . First, we set a bound h_{\max} on aggregate constraint violation, so that each point $y \in \mathcal{F}$ satisfies $h_X(y) < h_{\max}$. Second, we include only infeasible points in the filter and track feasible points separately. This is done in order to avoid a problem with what Fletcher and Leyffer [15] refer to as “blocking entries”, in which a feasible filter point with lower function value than a nearby local minimum prevents convergence to both that minimum and a global minimum. Tracking feasible points outside of the filter circumvents this uncommon but plausible scenario. With these two modifications, the following terminology is now provided.

Definition 4.3 *A point x is said to be filtered by a filter \mathcal{F} if any of the following properties hold:*

1. *There exists a point $y \in \mathcal{F}$ such that $y \preceq x$,*
2. *$h_X(x) \geq h_{\max}$,*
3. *$h_X(x) = 0$ and $f(x) \geq f^F$, where f^F is the objective function value of the best feasible point found thus far.*

The point x is said to be unfiltered by \mathcal{F} if it is not filtered by \mathcal{F} .

Thus, the set of unfiltered points, denoted by $\overline{\mathcal{F}}$, is given by

$$\overline{\mathcal{F}} = \bigcup_{x \in \mathcal{F}} \{y : y \succeq x\} \cup \{y : h_X(y) \geq h_{\max}\} \cup \{y : h_X(y) = 0, f(y) \geq f^F\}. \quad (9)$$

Observe that, with this notation, if a new trial point has the same function values as those of any point in the filter, then the trial point is filtered. Thus, only the first point with such values is accepted into the filter.

4.2 Description of the Algorithm

For the new class of algorithms, at each iteration k , the poll center p_k is chosen as either the incumbent best feasible point p_k^F or the incumbent least infeasible point p_k^I . For a given poll center p_k , the poll set $P_k(p_k)$ is defined in equation (4).

Because the filter seeks a better point with respect to either of the two functions (the objective function f and the constraint violation function h_X), a change must be made to the rule for selecting discrete neighbors, about which to perform an EXTENDED POLL step. Recall that in the MVPS algorithm, extended polling is performed around any discrete neighbor whose objective function value is sufficiently close to that of the current iterate (*i.e.*, “almost” an improved mesh point). With the addition of nonlinear constraints to the problem, we require a notion of a discrete neighbor “almost” generating a new incumbent best feasible point or least infeasible point.

While this issue has by no means a single workable approach, the implementation here has the desirable property of being a generalization of the MVPS algorithm. At iteration k , let $f_k^F = f(p_k^F)$ denote the objective function value of the incumbent best feasible point. If no feasible point exists, we set $f_k^F = \infty$. Similarly, let $h_k^I = h_X(p_k^I) > 0$ be the constraint violation function value of the incumbent least infeasible point. If no such point exists, we set $h_k^I = h_{\max}$ and $f_k^I = -\infty$, where $f_k^I = f(p_k^I)$ is the objective function value of the least infeasible point. Given current poll center p_k and user-specified extended poll triggers $\xi_k^f \leq \xi > 0$ and $\xi_k^h \leq \xi > 0$ for f and h , respectively (where ξ is a positive constant), we perform an EXTENDED POLL step around any discrete neighbor $y_k \in \mathcal{N}(p_k)$ satisfying either $0 < h_k^I < h_X(y_k) < \min(h_k^I + \xi_k^h, h_{\max})$, or $h_X(y_k) = 0$ with $f_k^F < f(y_k) < f_k^F + \xi_k^f$. The extended poll triggers ξ_k^f and ξ_k^h can also be set according to the categorical variable values associated with the current poll center, but this dependency is not included in the notation, so as not to obfuscate the ideas presented here.

Similar to the MVPS algorithm described in Section 3, the EXTENDED POLL STEP generates a sequence of EXTENDED POLL centers $\{y_k^j\}_{j=0}^{J_k}$, beginning with $y_k^0 = y_k$ and ending with *extended poll endpoint*, $y_k^{J_k} = z_k$.

Thus, at iteration k , the set of all points evaluated in the EXTENDED POLL step, denoted $\mathcal{X}_k(\xi_k^f, \xi_k^h)$, is

$$\mathcal{X}_k(\xi_k^f, \xi_k^h) = \bigcup_{y \in \mathcal{N}_k^f \cup \mathcal{N}_k^h} \mathcal{E}(y) \quad (10)$$

where $\mathcal{E}(y)$ denotes the set of extended poll points, and

$$\mathcal{N}_k^f = \{y \in \mathcal{N}(p_k) : h_X(y) = 0, f_k^F \leq f(y) \leq f_k^F + \xi_k^f\}, \quad (11)$$

$$\mathcal{N}_k^h = \{y \in \mathcal{N}(p_k) : 0 < h_k^I < h_X(y) < \min(h_k^I + \xi_k^h, h_{\max})\}. \quad (12)$$

The set of trial points is defined as $T_k = S_k \cup P_k(p_k) \cup \mathcal{N}(p_k) \cup \mathcal{X}_k(\xi_k^f, \xi_k^h)$, where S_k is the finite set of mesh points evaluated during the SEARCH step.

The addition of the filter complicates our notions of success or failure of the iteration in finding a desirable iterate. The following definitions now define the two outcomes of the SEARCH, POLL, and EXTENDED POLL steps.

Definition 4.4 Let T_k denote the set of trial points to be evaluated at iteration k , and let $\bar{\mathcal{F}}_k$ denote the set of filtered points described by (9). A point $y \in T_k$ is said to be an unfiltered point if $y \notin \bar{\mathcal{F}}_k$.

Definition 4.5 Let $P_k(p_k)$ denote the poll set centered at the point p_k , and let $\bar{\mathcal{F}}_k$ denote the set of filtered points described by (9). The point p_k is said to be a mesh isolated filter point if $P_k(p_k) \cup \mathcal{N}(p_k) \cup \mathcal{X}(\xi_k^f, \xi_k^h) \subset \bar{\mathcal{F}}_k$.

Figure 1 is a depiction of a filter on a bi-loss graph, in which the best feasible and least infeasible solutions are indicated, and the feasible solutions lie on the vertical axis (labelled f). Dashed lines indicate the areas for which an EXTENDED POLL step is triggered. If a feasible discrete neighbor has an objective function value that lies on $(f_k^F, f_k^F + \epsilon_k^f)$ (i.e., higher on the axis than the current incumbent, but lower than the horizontal dashed line), an EXTENDED POLL step is performed around this discrete neighbor. Similarly, an EXTENDED POLL step is performed if an infeasible discrete neighbor has a constraint violation function value that lies on $(h_k^F, h_k^F + \epsilon_k^h)$ (i.e., it lies to the right of the current least infeasible solution, but left of the vertical dashed line).

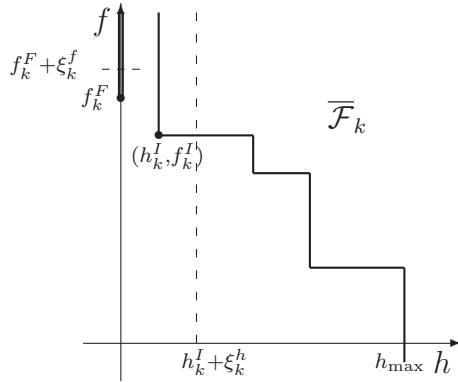


Figure 1: MVP Filter and Extended Poll Triggers.

The goal of each iteration is to find an unfiltered point, but the details of when to continue an EXTENDED POLL step must be generalized from the simple decrease condition in f under which the MVPS algorithm operates. More specifically, if the EXTENDED POLL step finds an unfiltered point, it is added to the filter, the poll center is updated (if appropriate), and the mesh is coarsened according to the rule in (6). If the EXTENDED POLL step fails to find a new point y satisfying $y \in \mathcal{N}_k^f \cup \mathcal{N}_k^h$, then the current incumbent poll center p_k is declared

to be a mesh isolated filter point, the current poll center is retained, and the mesh is refined according to the rule in (7).

Finally, we treat the case in which extended poll points are filtered, yet still belong to \mathcal{N}_k^f or \mathcal{N}_k^h . To do so, we establish the notion of a temporary *local filter*. At iteration k , for each discrete neighbor y_k , a local filter $\mathcal{F}_k^L(y_k)$ is constructed relative to the current EXTENDED POLL step and initialized only with the point y_k and $h_{\max}^L = \min(h_k^I + \xi_k^h, h_{\max})$. As with the MVPS algorithm, the extended poll sequence $\{y_k^j\}_{j=1}^{J_k}$ begins with $y_k^0 = y_k$ and ends with $z_k = y_k^{J_k}$, where each y_k^j is the poll center of the local filter – chosen either as the best feasible or least infeasible point, relative to the local filter. Extended polling with respect to y_k proceeds, with the local filter being updated as appropriate, until no more unfiltered mesh points can be found with respect to the new local filter, or until an unfiltered point is found with respect to the main filter. When either of these conditions is satisfied, the EXTENDED POLL step ends, and the main filter is appropriately updated with the points of the local filter, which is then discarded. The mesh size parameter Δ_k , which is constant throughout the step, is then updated, depending on whether an unfiltered point (with respect to the main filter) has been found.

The EXTENDED POLL step and and Filter-MVPS (FMVPS) Algorithm are summarized in Figures 2 and 3.

EXTENDED POLL Step at Iteration k

Input: Current poll center p_k , filter \mathcal{F}_k , and extended poll triggers ξ_k^f and ξ_k^h .

For each discrete neighbor $y_k \in \mathcal{N}_k^f \cup \mathcal{N}_k^h$ (see (11) and (12)), do the following:

- Initialize local filter \mathcal{F}_k^L with y_k and $h_{\max}^L = \min\{h_k^I + \xi_k^h, h_{\max}\}$. Set $y_k^0 = y_k$.
- For $j = 0, 1, 2, \dots$
 1. Evaluate f and h_X at points in $P_k(y_k^j)$ until a point w is found that is unfiltered with respect to \mathcal{F}_k^L , or until done.
 2. If no point $w \in P_k(y_k^j)$ is unfiltered with respect to \mathcal{F}_k^L , then go to **Next**.
 3. If a point w is unfiltered with respect to \mathcal{F}_k , set $x_{k+1} = w$ and **Quit**.
 4. If w is filtered with respect to \mathcal{F}_k , but unfiltered with respect to \mathcal{F}_k^L , then update \mathcal{F}_k^L to include w , and compute new extended poll center y_k^{j+1} .
- **Next:** Discard \mathcal{F}_k^L and process next $y_k \in \mathcal{N}_k^f \cup \mathcal{N}_k^h$.

Figure 2: Extended Poll Step for the FMVPS Algorithm

Filter Mixed Variable Generalized Pattern Search – FMVPS

Initialization: Let x_0 be an undominated point of a set of initial solutions. Include all these points in the filter \mathcal{F}_0 , with $h_{\max} > h_X(x_0)$. Fix $\xi > 0$ and $\Delta_0 > 0$.

For $k = 0, 1, 2, \dots$, perform the following:

1. Choose a poll center $p_k \in \{p_k^F, p_k^I\}$, and update the extended poll triggers $\xi_k^f \geq \xi$ and $\xi_k^h \geq \xi$.
2. Set the incumbent values $f_k^F = f(p_k^F), h_k^I = h_X(p_k^I), f_k^I = f(p_k^I)$.
3. **SEARCH step:** Employ some finite strategy seeking an unfiltered mesh point $x_{k+1} \notin \overline{\mathcal{F}}_k$.
4. **POLL step:** If the SEARCH step did not find an unfiltered point, evaluate f and h at points in the poll set $P_k(p_k) \cup \mathcal{N}(p_k)$ until an unfiltered mesh point $x_{k+1} \notin \overline{\mathcal{F}}_k$ is found, or until done.
5. **EXTENDED POLL step:** If SEARCH and POLL did not find an unfiltered point, execute the algorithm in Figure 2 to continue looking for $x_{k+1} \notin \overline{\mathcal{F}}_k$.
6. **Update:** If SEARCH, POLL, or EXTENDED POLL finds an unfiltered point, Update filter \mathcal{F}_{k+1} with x_{k+1} , and set $\Delta_{k+1} \geq \Delta_k$ according to (6); Otherwise, set $\mathcal{F}_{k+1} = \mathcal{F}_k$, and set $\Delta_{k+1} < \Delta_k$ according to (7).

Figure 3: FMVPS Algorithm

5 Convergence Analysis

The convergence properties of the new algorithm are now presented. First, the behavior of the mesh size parameter Δ_k will be shown to have the same behavior as in previous algorithms, and a general characterization of limit points of certain subsequences is given. Results for the constraint violation function and for the objective function follow, similar to those found in [8]. Finally, stronger results for a more specific implementation of the new algorithm are provided. These mimic those found in [6], but apply to the more general MVP problem with nonlinear constraints. We should note that many of the results presented here are significantly different than the original presentation in [1].

We make the following assumptions, consistent with those of previous GPS algorithms:

- A1:** All iterates $\{x_k\}$ produced by the algorithm lie in a compact set.
- A2:** For each fixed x^d , the corresponding set of directions $D^i = G_i Z_i$, as defined in (2), includes tangent cone generators for every point in $X^c(x^d)$.
- A3:** If x is a poll center, or an extended poll center, the rule for selecting directions $D_k(x)$ conforms to X^c for some $\epsilon > 0$ (see Definition 3.1).
- A4:** The discrete neighbors always lie on the mesh; i.e., $\mathcal{N}(x_k) \subset M_k$ for all k .

5.1 Mesh Size Behavior and Limit Points

The behavior of the mesh size was originally characterized for unconstrained problems by Torczon [28], independent of the smoothness of the objective function. It was extended to MVP problems by Audet and Dennis [6], who later adapted the proof to provide a lower bound on the distance between mesh points at each iteration [7]. The proofs here are straightforward extensions of the latter work to MVP problems. The first lemma provides the lower bound on the distance between any two mesh points whose continuous variable values do not coincide, while the second lemma shows that the mesh size parameter is bounded above. The theorem that follows shows the key result that $\liminf_{k \rightarrow +\infty} \Delta_k = 0$.

Lemma 5.1 *For any integer $k \geq 0$, let u and v be any distinct points in the mesh M_k such that $u^d = v^d$. Then for any norm for which all nonzero integer vectors have norm at least 1,*

$$\|u^c - v^c\| \geq \frac{\Delta_k}{\|G_i^{-1}\|}.$$

where the index i corresponds to the discrete variable values of u and v .

Proof. Using (4), we let $u^c = x_k^c + \Delta_k D^i z_u$ and $v^c = x_k^c + \Delta_k D^i z_v$ define the continuous part of two distinct points on M_k with both $z_u, z_v \in \mathbb{Z}_+^{|D^i|}$. Furthermore, since we assume that u and v are distinct with $u^d = v^d$, we must have $u^c \neq v^c$, and thus $z_u \neq z_v$. Then

$$\|u^c - v^c\| = \Delta_k \|D^i(z_u - z_v)\| = \Delta_k \|G_i Z_i(z_u - z_v)\| \geq \Delta_k \frac{\|Z_i(z_u - z_v)\|}{\|G_i^{-1}\|} \geq \frac{\Delta_k}{\|G_i^{-1}\|},$$

the last inequality because $Z_i(z_u - z_v)$ is a nonzero integer vector with norm greater than or equal to one. ■

Lemma 5.2 *There exists a positive integer r^u such that $\Delta_k \leq \Delta_0 \tau^{r^u}$ for any integer $k \geq 0$.*

Proof. Under Assumption A1, the discrete variables can only take on a finite number of values in $L_X(x_0)$. Let i_{\max} denote this number, and let $I = \{1, 2, \dots, i_{\max}\}$. Also under Assumption A1, for each $i \in I$, let Y_i be a compact set in \mathbb{R}^{n^c} containing all GPS iterates whose discrete variable values correspond to $i \in I$. Let $\gamma = \max_{i \in I} \text{diam}(Y_i)$ and $\beta = \min_{i \in I} \|G_i^{-1}\|$, where diam indicates the maximum distance between any two points. If $\Delta_k > \gamma\beta$, then Lemma 5.1 (with $v = x_k$) ensures that any trial point $u \in M_k$ either satisfies $u^c = x_k^c$ or would have lied outside of $\bigcup_{i \in I} Y_i$. Then if $\Delta_k > \gamma\beta$, no more than i_{\max} successful iterations will occur before Δ_k falls below $\gamma\beta$. Thus, Δ_k is bounded above by $\gamma\beta(\tau^{m_{\max}})^{i_{\max}}$, and the result follows by setting r^u large enough so that $\Delta_0\tau^{r^u} \geq \gamma\beta(\tau^{m_{\max}})^{i_{\max}}$. ■

Theorem 5.3 *The mesh size parameters satisfy $\liminf_{k \rightarrow +\infty} \Delta_k = 0$.*

Proof. (Torczon [28]) Suppose by way of contradiction that there exists a negative integer r^ℓ such that $0 < \Delta_0\tau^{r^\ell} \leq \Delta_k$ for all integer $k \geq 0$. Combining (8) with Lemma 5.2 implies that for any integer $k \geq 0$, r_k takes its value from among the integers of the finite set $\{r^\ell, r^\ell + 1, \dots, r^u\}$. Therefore, r_k and Δ_k can only take a finite number of values for all $k \geq 0$.

Since $x_{k+1} \in M_k$, (4) ensures that $x_{k+1}^c = x_k^c + \Delta_k D^i z_k$ for some $z_k \in \mathbb{Z}_+^{|D^i|}$ and $1 \leq i \leq i_{\max}$. By repeatedly applying this equation and substituting $\Delta_k = \Delta_0\tau^{r_k}$, it follows that, for any integer $N \geq 1$,

$$\begin{aligned} x_N^c &= x_0^c + \sum_{k=1}^{N-1} \Delta_k D^i z_k \\ &= x_0^c + \Delta_0 D^i \sum_{k=1}^{N-1} \tau^{r_k} z_k = x_0^c + \frac{p^{r^\ell}}{q^{r^u}} \Delta_0 D^i \sum_{k=1}^{N-1} p^{r_k - r^\ell} q^{r^u - r_k} z_k, \end{aligned}$$

where p and q are relatively prime integers satisfying $\tau = \frac{p}{q}$. Since $p^{r_k - r^\ell} q^{r^u - r_k} z_k$ is an integer for any k , it follows that the continuous part of all iterates having the same discrete variable values lies on the translated integer lattice generated by x_0^c and the columns of $\frac{p^{r^\ell}}{q^{r^u}} \Delta_0 D^i$. Moreover, the discrete part of all iterates also lies on the integer lattice $X^d \subset \mathbb{Z}^{n^d}$.

Therefore, since all iterates belong to a compact set, there must be only a finite number of different iterates, and thus one of them must be visited infinitely many times. Therefore, the mesh coarsening rule in (6) is only applied finitely many times, and the mesh refining rule in (7) is applied infinitely many times. This contradicts the hypothesis that $\Delta_0\tau^{r^\ell}$ is a lower bound for the mesh size parameter. ■

These results show the necessity of forcing the set of directions to satisfy $D^i = G_i Z_i$. Under Assumption A1, this ensures that the mesh has only a finite number of points in X , which means that there can only be a finite number of consecutive unfiltered mesh points.

Assumption A2 is included to simply ensure that this construction is maintained in the presence of linear constraints. Audet and Dennis [7] provide an example in which a different construction yields a mesh that is dense in X . In this case, Lemma 5.1 cannot be satisfied, and convergence of Δ_k to zero is not guaranteed. A sufficient condition for Assumption A2 to hold is that $G_i = I$ for each $i = 1, 2, \dots, i_{\max}$ and that the coefficient matrix A is rational [23].

We should note also that the rationality of τ is essential for convergence. Audet [4] gives an example in which an irrational value for τ generates a sequence satisfying $\liminf_{k \rightarrow +\infty} \Delta_k > 0$.

5.2 Refining Subsequences

Since Δ_k shrinks only at iterations in which no mesh isolated filter point is found, Theorem 5.3 guarantees that the Filter-MVPS algorithm has infinitely many such iterations. We are particularly interested in subsequences of iterates that correspond to these points. We now include the following two useful definitions.

Definition 5.4 *A subsequence of mesh isolated filter points $\{p_k\}_{k \in K}$ (for some subset of indices K) is said to be a refining subsequence if $\{\Delta_k\}_{k \in K}$ converges to zero.*

Definition 5.5 *Let $\{v_k\}_{k \in K}$ be either a refining subsequence or a corresponding subsequence of extended poll endpoints, and let \hat{v} be a limit point of the subsequence. A direction $d \in D$ is said to be a limit direction of \hat{v} if $v_k + \Delta_k(d, 0)$ belongs to X and is filtered for infinitely many $k \in K$.*

The following theorem of Audet and Dennis [6] establishes the existence of limit points of specific subsequences of interest. Its proof, which can be found in [6], is omitted.

Theorem 5.6 *There exists a point $\hat{p} \in \{x \in X : f(x) \leq f(x_0)\}$ and a refining subsequence $\{p_k\}_{k \in K}$ (with associated index set K) such that $\lim_{k \in K} p_k = \hat{p}$. Moreover, if \mathcal{N} is continuous at \hat{p} , then there exists $\hat{y} \in \mathcal{N}(\hat{p})$ and $\hat{z} = (\hat{z}^c, \hat{y}^d) \in X$ such that*

$$\lim_{k \in K} y_k = \hat{y} \quad \text{and} \quad \lim_{k \in K} z_k = \hat{z},$$

where each $z_k \in X$ is the endpoint of the EXTENDED POLL step initiated at $y_k \in \mathcal{N}(p_k)$.

The notation in Theorem 5.6 describing specific subsequences and their limit points will be retained and used throughout the remainder of this paper.

5.3 Background for Optimality Results

In this subsection, we provide some additional background material, based on the ideas of the Clarke calculus, along with a new definition and theorem that will be used in the convergence theorems. Some of these ideas have been used in proofs by Audet and Dennis [7, 8] in the context of certain limit points of the GPS algorithm, and the new definition allows use to generalize slightly their hypotheses.

First, the following definitions from [12] are needed. They apply to any function $g : \mathbb{R}^n \rightarrow \mathbb{R}$ that is Lipschitz near a point $x \in \mathbb{R}^n$.

- The *generalized directional derivative* of g at x in the direction v is given by

$$g^\circ(x; v) := \limsup_{y \rightarrow x, t \downarrow 0} \frac{g(y + tv) - g(y)}{t},$$

where t is a positive scalar.

- The *generalized gradient* of g at x is the set

$$\partial g(x) := \{\zeta \in \mathbb{R}^n : g^\circ(x; v) \geq v^T \zeta \text{ for all } v \in \mathbb{R}^n\}.$$

- g is *strictly differentiable* at x if, for all $v \in \mathbb{R}^n$,

$$\lim_{y \rightarrow x, t \downarrow 0} \frac{g(y + tv) - g(y)}{t} = \nabla g(x)^T v.$$

The following is a generalization of the previous definition.

Definition 5.7 Let X be a convex subset of \mathbb{R}^n . Let $T_X(x)$ denote the tangent cone to X at $x \in X$. A function g is said to be strictly differentiable with respect to X at $x \in X$ if, for all $v \in T_X(x)$,

$$\lim_{y \rightarrow x, y \in X, t \downarrow 0} \frac{g(y + tv) - g(y)}{t} = \nabla g(x)^T v.$$

Theorem 5.8 below essentially establishes first-order necessary conditions for optimality with respect to the continuous variables in a mixed variable domain. The assumptions on g given here are slightly weaker than the strict differentiability assumption used in [7] to establish first-order results for GPS limit points – but only in the presence of linear constraints. Without linear constraints, Definition 5.7 clearly reduces to that of strict differentiability.

However, we first introduce new notation, so that $g'(x; (d, 0))$ denotes the directional derivative at x with respect to the continuous variables in the direction $d \in \mathbb{R}^{n^c}$ (i.e., while holding the discrete variables constant – hence the $0 \in \mathbb{Z}^{n^d}$), $g^\circ(x; (d, 0))$ denotes the Clarke generalized directional derivative at x with respect to the continuous variables, and $\partial^c g(x)$ represents the generalized gradient of f at x with respect to the continuous variables. This convention is used throughout Section 5.

Theorem 5.8 Let $x = (x^c, x^d) \in X \subseteq \mathbb{R}^{n^c} \times \mathbb{Z}^{n^d}$. Suppose the function g is strictly differentiable with respect to X^c at x . If $D \in \mathbb{R}^{n^c}$ positively spans the tangent cone $T_{X^c}(x)$, and if $g^\circ(x; (d, 0)) \geq 0$ for all $d \in D \cap T_{X^c}(x)$, then $\nabla^c g(x)^T v \geq 0$ for all $v \in T_{X^c}(x)$. Thus, x is a KKT point of g with respect to the continuous variables. Moreover, if $X^c = \mathbb{R}^{n^c}$ or if x^c lies in the interior of X^c , then f is strictly differentiable at x with respect to the continuous variables and $0 = \nabla^c g(x) \in \partial^c g(x)$.

Proof. Under the hypotheses given, let D be a set of vectors that positively spans $T_{X^c}(x)$, and let $v \in X^c$ be arbitrary. Then $v = \sum_{i=1}^{|D|} \alpha_i d_i$ for some $\alpha_i \geq 0$ and $d_i \in D$, $i = 1, 2, \dots, |D|$. Then

$$\nabla^c g(x)^T v = \sum_{i=1}^{|D|} \alpha_i \nabla^c g(x)^T d_i = \sum_{i=1}^{|D|} \alpha_i g^\circ(x; (d_i, 0)) \geq 0,$$

since all the terms of the final sum are nonnegative.

If $X^c = \mathbb{R}^{n^c}$, or if x^c lies in the interior of X^c , then $T_{X^c}(x) = \mathbb{R}^{n^c}$ and g is strictly differentiable at x . Since we have $\nabla^c g(x)^T v \geq 0$ for all $v \in \mathbb{R}^{n^c}$, including $-v$, we also have $\nabla^c g(x)^T v \leq 0$ for all $v \in \mathbb{R}^{n^c}$. Therefore, $0 = \nabla^c g(x) \in \partial^c g(x)$, (the last step because $\partial^c f(x)$ always contains $\nabla^c g(x)$, if it exists). ■

5.4 Results for the Constraint Violation Function

Theorem 5.6 defines and establishes existence of the limit points \hat{p} , \hat{y} , and \hat{z} . While the next result applies to more general limit points of the algorithm, the remainder of the results in this section apply to these specific limit points. This format will be repeated in Section 5.5 as well. This first result, which is similar to a theorem in [7] for f , requires a very mild condition on h . Note that this result will not hold for f without an additional assumption because there is no guarantee that any subsequence of objective function values is nonincreasing.

Theorem 5.9 If h is lower semi-continuous with respect to the continuous variables at a limit point \bar{p} of poll centers $\{p_k\}$, then $\lim_k h(p_k)$ exists and is greater than or equal to $h(\bar{p}) \geq 0$. If h is continuous at every limit point of $\{p_k\}$, then every limit point has the same function value.

Proof. If $h(\bar{p}) = 0$, the result follows trivially. Now let $h(\bar{p}) > 0$. Then \bar{p} is a limit point of a sequence of least infeasible points p_k^I , which is monotonically nonincreasing. Since h is lower semi-continuous at \bar{p} , we know that for any subsequence $\{p_k\}_{k \in K}$ of poll centers that converges to \bar{p} , $\liminf_{k \in K} h(p_k) \geq h(\bar{p}) \geq 0$. But the subsequence of constraint violation function values at p_k^I is a subsequence of a nonincreasing sequence. Thus, the entire sequence is also bounded below by $h(\bar{p})$, and so it converges. ■

We now characterize the limit points of Theorem 5.6 with respect to the constraint violation function h . The following theorem establishes the local optimality of h at \hat{p} with respect to its discrete neighbors. The short proof is nearly identical to one in [6].

Theorem 5.10 *Let \hat{p} and $\hat{y} \in \mathcal{N}(\hat{p})$ be defined as in the statement of Theorem 5.6, with \mathcal{N} continuous at \hat{x} . If h is lower semi-continuous at \hat{p} with respect to the continuous variables and continuous at \hat{y} with respect to the continuous variables, then $h(\hat{p}) \leq h(\hat{y})$.*

Proof. From Theorem 5.6, we know that $\{p_k\}_{k \in K}$ converges to \hat{p} and $\{y_k\}_{k \in K}$ converges to \hat{y} . Since $k \in K$ ensures that $\{p_k\}_{k \in K}$ are mesh isolated poll centers, we have $h(p_k) \leq h(y_k)$ for all $k \in K$, and by the assumptions of continuity and lower semi-continuity, we have $h(\hat{p}) \leq \lim_{k \in K} h(p_k) \leq \lim_{k \in K} h(y_k) = h(\hat{y})$. ■

The next two results establish a directional optimality condition for h at \hat{p} and at certain \hat{z} with respect to the continuous variables.

Theorem 5.11 *Let \hat{p} be a limit point of a refining subsequence. Under Assumptions A1–A4, if h is Lipschitz near \hat{p} with respect to the continuous variables, then $h^\circ(\hat{p}; (d, 0)) \geq 0$ for all limit directions $d \in D(\hat{p})$ of \hat{p} .*

Proof. Let $\{p_k\}_{k \in K}$ be a refining subsequence with limit point \hat{p} and let $d \in D(\hat{p})$ be a limit direction of \hat{p} . From the definition of the generalized directional derivative [12], we have

$$h^\circ(\hat{p}; (d, 0)) = \limsup_{y \rightarrow \hat{p}, t \downarrow 0} \frac{h(y + t(d, 0)) - h(y)}{t} \geq \limsup_{k \in K} \frac{h(p_k + \Delta_k(d, 0)) - h(p_k)}{\Delta_k}.$$

The function h is Lipschitz, hence finite, near \hat{p} . Since points that are infeasible with respect to X are not evaluated by the algorithm, the assumption of d being a limit direction of \hat{p} ensures that infinitely many right-hand quotients are defined. All of these quotients must be nonnegative, or else the corresponding POLL step would have found an unfiltered point, a contradiction. ■

Theorem 5.12 *Let $\hat{p}, \hat{y} \in \mathcal{N}(\hat{p})$, and \hat{z} be defined as in the statement of Theorem 5.6, with \mathcal{N} continuous at \hat{p} , and let $\xi > 0$ denote a lower bound on the extended poll triggers ξ_k^f and ξ_k^h for all k . If $h(\hat{y}) < h(\hat{p}) + \xi$ and h is Lipschitz near \hat{z} with respect to the continuous variables, then $h^\circ(\hat{z}; (d, 0)) \geq 0$ for all limit directions $d \in D(\hat{z})$ of \hat{z} .*

Proof. From the definition of the generalized directional derivative [12], we have

$$h^\circ(\hat{z}; (d, 0)) = \limsup_{y \rightarrow \hat{z}, t \downarrow 0} \frac{h(y + t(d, 0)) - f(y)}{t} \geq \limsup_{k \in K} \frac{h(z_k + \Delta_k(d, 0)) - h(z_k)}{\Delta_k}.$$

Now, h is Lipschitz, hence finite, near \hat{z} . Since $h(\hat{y}) < h(\hat{p}) + \xi$ ensures that extended polling was triggered around $y_k \in \mathcal{N}(p_k)$ for all sufficiently large $k \in K$, and since d is a limit

direction of \hat{z} , it follows that $z_k + \Delta_k(d, 0) \in X$ infinitely often in K , and infinitely many of the right-hand quotients are defined. All of these quotients must be nonnegative, since for $k \in K$, z_k is an extended poll endpoint. ■

For bound or linear constraints, in order to guarantee the existence of limit directions, for which Theorem 5.11 applies, each $D^i \subset D$, $i = 1, 2, \dots, i_{\max}$ is constructed in accordance with the algorithm given in [23] to generate a sufficiently rich set of directions to ensure conformity to X^c (see Definition 3.1), consistent with Assumption A3.

The next two key theorems establish conditions on h at \hat{p} and certain \hat{z} to satisfy a first-order optimality condition with respect to the continuous variables.

Theorem 5.13 *Let \hat{p} be the limit of a refining subsequence with limit directions $D(\hat{p})$, and suppose h is strictly differentiable with respect to X^c at \hat{p} . Then under Assumptions A1–A3, $\nabla^c h(\hat{p})^T w \geq 0$ for all $w \in T_{X^c}(\hat{p})$. Moreover, if $X^c = \mathbb{R}^{n^c}$, or if \hat{p} lies in the interior of X^c , then $0 = \nabla^c h(\hat{p}) \in \partial^c h(\hat{p})$.*

Proof. Since Assumption A3 ensures that the rule for selecting $D_k(p_k)$ conforms to X^c for some $\epsilon > 0$, and since there are finitely many linear constraints, $D_k(p_k) \rightarrow D(\hat{p})$, and $D(\hat{p})$ positively spans $T_{X^c}(\hat{p})$. Theorem 5.11 guarantees that $h^\circ(\hat{p}, (d, 0)) \geq 0$ for all $d \in D(\hat{p})$, and the result follows directly from Theorem 5.8. ■

Theorem 5.14 *Let \hat{p} , $\hat{y} \in \mathcal{N}(\hat{p})$, and \hat{z} be defined as in the statement of Theorem 5.6, with \mathcal{N} continuous at \hat{p} , and let $\xi > 0$ denote a lower bound on the extended poll triggers ξ_k^f and ξ_k^h for all k . Let $D(\hat{z})$ denote the limit directions of \hat{z} , and suppose h is strictly differentiable with respect to X^c at \hat{z} . If $h(\hat{y}) < h(\hat{p}) + \xi$, then under Assumptions A1–A4, $\nabla^c h(\hat{z})^T w \geq 0$ for all $w \in T_{X^c}(\hat{z})$. Furthermore, if $X^c = \mathbb{R}^{n^c}$ or \hat{z}^c lies in the interior of X^c , then $0 = \nabla^c h(\hat{z}) \in \partial^c h(\hat{z})$.*

Proof. Since Assumption A3 ensures that the rule for selecting $D_k(z_k)$ conforms to X^c for some $\epsilon > 0$, and since there are finitely many linear constraints, $D_k(z_k) \rightarrow D(\hat{z})$, and $D(\hat{z})$ positively spans $T_{X^c}(\hat{z})$. Theorem 5.12 ensures that $h^\circ(\hat{z}; (d, 0)) \geq 0$ for all $d \in D(\hat{z})$, and the result follows directly from Theorem 5.8. ■

5.5 Results for the Objective Function

We now address the properties of certain limit points with respect to the objective function f . Unfortunately, in order to obtain results for f that are similar to those for h , an additional hypothesis must be added to most of the theorems that follow. Additionally, convergence to a KKT point (with respect to the continuous variables) cannot be guaranteed, but we will show a similar result to that of [8], in which a cone is identified whose polar contains the normal cone.

The first result, under very mild conditions, is similar to Theorem 5.9, but requires polling to be centered at the best feasible point at all but finitely many iterations.

Theorem 5.15 *Under Assumption A1, there exists at least one limit point \bar{p} of the iteration sequence $\{p_k\}$ of poll centers. If f is lower semi-continuous at \bar{p} with respect to the continuous variables, h is continuous at \bar{p} with respect to the continuous variables, and $p_k = p_k^F$ for all but finitely many k , then $\lim_k f(p_k)$ exists and is greater than or equal to $f(\bar{p})$, which is finite. If f is continuous at every limit point of $\{p_k\}$, then every limit point has the same function value.*

Proof. First, $p_k = p_k^F$, hence $h(p_k) = 0$, for all but finitely many k . Thus, f is nonincreasing, for all sufficiently large k . Since f is lower semi-continuous at \bar{p} , we know that for any subsequence $\{p_{k_j}\}_{j \in K}$ of poll centers converging to \bar{p} , $\liminf_{j \in K} f(p_{k_j}) \geq f(\bar{p})$. But the subsequence of function values is a subsequence of a nonincreasing sequence (for sufficiently large k). Thus, for sufficiently large k , the sequence is also bounded below by $f(\bar{p})$, and so it converges. ■

The remainder of this section contains results for the limit points described by Theorem 5.6. Each theorem contains an additional necessary hypothesis that, for infinitely many iterations of the specified subsequence, trial points must be filtered by the poll center (or extended poll endpoint), rather than a different filter point.

The following result, which is similar to Theorem 5.10, establishes optimality conditions with respect to the discrete set of neighbors.

Theorem 5.16 *Let \hat{p} and $\hat{y} \in \mathcal{N}(\hat{p})$ be defined as in the statement of Theorem 5.6, with \mathcal{N} continuous at \hat{x} . If f is lower semi-continuous at \hat{p} and \hat{y} with respect to the continuous variables, and if $f(p_k) \leq f(y_k)$ for infinitely many $k \in K$, then $f(\hat{p}) \leq f(\hat{y})$.*

Proof. From Theorem 5.6, we know that $\{p_k\}_{k \in K}$ converges to \hat{p} and $\{y_k\}_{k \in K}$ converges to \hat{y} . Without loss of generality, we may assume that $h(p_k) < h_{\max}$ for all $k \in K$. Then, since $f(p_k) \leq f(y_k)$ for infinitely many $k \in K$, we have by the assumptions of continuity and lower semi-continuity, that $f(\hat{p}) \leq \lim_{k \in K} f(p_k) \leq \lim_{k \in K} f(y_k) = f(\hat{y})$. ■

The next two results establish conditions under which certain Clarke generalized directional derivatives are nonnegative. The first theorem applies to \hat{p} , while the second applies to some \hat{z} . As before, these theorems require the additional hypothesis that the incumbent poll center or extended poll endpoint, rather than a different filter point, filter the trial points infinitely often in the subsequence.

Theorem 5.17 *Let \hat{p} be a limit point of a refining subsequence $\{p_k\}_{k \in K}$, and let $d \in D$ be a limit direction of \hat{p} . Under Assumptions A1–A4, if f is Lipschitz near \hat{p} with respect to the continuous variables, and $f(p_k) \leq f(p_k + \Delta_k(d, 0))$ for infinitely many $k \in K$, then $f^\circ(\hat{p}; (d, 0)) \geq 0$.*

Proof. From the definition of the generalized directional derivative [12], we have that

$$f^\circ(\hat{p}; (d, 0)) = \limsup_{y \rightarrow \hat{p}, t \downarrow 0} \frac{f(y + t(d, 0)) - f(y)}{t} \geq \limsup_{k \in K} \frac{f(p_k + \Delta_k(d, 0)) - f(p_k)}{\Delta_k},$$

which is nonnegative, since an infinite number of terms in the right-hand quotient are non-negative. \blacksquare

Theorem 5.18 Let $\hat{p}, \hat{y} \in \mathcal{N}(\hat{p})$, \hat{z} , and z_k be defined as in the statement of Theorem 5.6, with \mathcal{N} continuous at \hat{p} , and let $d \in D$ be a limit direction for \hat{z} . Suppose that $f(\hat{y}) < f(\hat{p}) + \xi$, where $\xi > 0$ is a lower bound on the extended poll triggers ξ_k^f and ξ_k^h for all k . Under Assumptions A1–A4, if f is Lipschitz near \hat{z} with respect to the continuous variables, and $f(z_k) \leq f(z_k + \Delta_k(d, 0))$ for infinitely many $k \in K$, then $f^\circ(\hat{z}; (d, 0)) \geq 0$.

Proof. From the definition of the generalized directional derivative [12], we have that

$$f^\circ(\hat{z}; (d, 0)) = \limsup_{y \rightarrow \hat{z}, t \downarrow 0} \frac{f(y + t(d, 0)) - f(y)}{t} \geq \limsup_{k \in K} \frac{f(z_k + \Delta_k(d, 0)) - f(z_k)}{\Delta_k},$$

which is nonnegative, since an infinite number of terms in the right-hand quotient are non-negative. \blacksquare

The next two results describe the optimality conditions for f at \hat{p} and at certain \hat{z} under the assumptions of strict differentiability with respect to X^c . Once again, these theorems require that trial points be filtered by the poll center (rather than a different filter point) infinitely often in the subsequence.

As is the case with the Filter GPS algorithm, convergence to a KKT point cannot be guaranteed with respect to the continuous domain, since there is no guarantee that the negative gradient lies inside the normal cone; however, we specify a cone, whose polar contains the negative gradient.

Theorem 5.19 Let \hat{p} be a limit point of a refining subsequence $\{p_k\}_{k \in K}$, and let V_d be the cone generated by all limit directions $d \in D$ of \hat{p} , for which $f(p_k) \leq f(p_k + \Delta_k d)$ holds infinitely often. Suppose that f is strictly differentiable with respect to X^c at \hat{p} . Then under Assumptions A1–A4, $-\nabla^c f(\hat{p})$ belongs to the polar V_d° of V_d .

Proof. By Theorem 5.17, $f^\circ(\hat{p}; (d, 0)) \geq 0$ for all $d \in V_d$, and by Theorem 5.8, we have $\nabla^c f(\hat{p})^T w \geq 0$ for all $w \in V_d$. The result follows from the definition of a polar cone: $-\nabla^c f(\hat{p}) \in \{v \in \mathbb{R}^n : v^T w \leq 0 \forall w \in V_d\}$. \blacksquare

Theorem 5.20 Let $\hat{p}, \hat{y} \in \mathcal{N}(\hat{p})$, \hat{z} , and z_k be defined as in the statement of Theorem 5.6, with \mathcal{N} continuous at \hat{p} , and suppose that $f(\hat{y}) < f(\hat{p}) + \xi$, where $\xi > 0$ is a lower bound on the extended poll triggers ξ_k^f and ξ_k^h for all k . Let V_d be the cone generated by all limit directions $d \in D$ of \hat{z} , for which $f(z_k) \leq f(z_k + \Delta_k d)$ holds infinitely often. Suppose that f is strictly differentiable at with respect to X^c at \hat{p} . Then under Assumptions A1–A4, $-\nabla^c f(\hat{z})$ belongs to the polar V_d° of V_d .

Proof. By Theorem 5.18, $f^\circ(\hat{z}; (d, 0)) \geq 0$ for all $d \in V_d$, and by Theorem 5.8, we have $\nabla^c f(\hat{z})^T w \geq 0$ for all $w \in V_d$. The result follows from the definition of a polar cone: $-\nabla^c f(\hat{z}) \in \{v \in \mathbb{R}^n : v^T w \leq 0 \forall w \in V_d\}$. ■

Remark 5.21 *The additional hypothesis in Theorems 5.16–5.20 that the trial points be filtered by the current poll center infinitely often in the associated subsequence are automatically satisfied by either of the following two conditions:*

1. *The poll center (or extended poll center) is chosen to be the incumbent best feasible point (or best feasible point with respect to the local filter) infinitely often in the subsequence; i.e., $p_k = p_k^F$ (or alternatively $z_k = z_k^F$) for infinitely many $k \in K$. To see this for p_k , observe that $p_k = p_k^F$ infinitely often means that $h(p_k) = 0$ for infinitely often, and since these p_k are mesh isolated poll centers, $f(p_k) \leq f(p_k + \Delta_k d)$ for all limit directions $d \in D$ for \hat{p} . Note that $p_k = p_k^F$ is chiefly an algorithmic choice, rather than a problem-dependent condition.*
2. *The limit point is strictly feasible with respect to the nonlinear constraints C , and C is continuous at the limit point. This holds because these two conditions ensure that for all sufficiently large $k \in K$, $p_k = p_k^F$.* ■

Finally, we point out one other key result that we adapt from [8].

Theorem 5.22 *If h and f are strictly differentiable at poll center p_k with respect to the continuous variables, and if $\nabla^c f(p_k) \neq 0$, then there cannot be infinitely many consecutive iterations where p_k is a mesh isolated poll center.*

Proof. Let f and h be strictly differentiable at p_k with respect to the continuous variables, where $\nabla^c f(p_k) \neq 0$. Suppose that there are infinitely many iterations where p_k is a mesh isolated filter point. Let d be a direction associated with the (constant) subsequence of poll centers such that $\nabla^c f(p_k)^T d < 0$.

Since f is strictly differentiable at p_k with respect to the continuous variables, there exists an $\epsilon > 0$ such that either $h(p_k + \Delta(d, 0)) \leq h(p_k) < h_{\max}$, or $h(p_k + \Delta(d, 0)) > h(p_k)$, for all $0 < \Delta < \epsilon$.

If the first condition is satisfied, then for $\Delta_k < \epsilon$, the POLL step will find an unfiltered point, a contradiction. If the second condition is satisfied, then let \tilde{h} be the smallest value of

$$\{h(x) : h(x) > h(p_k), x \in \mathcal{F}_k\} \cup \{h_{\max}\},$$

and let \tilde{f} be the corresponding objective function value; i.e., either $\tilde{f} = f(\tilde{x})$ for the vector $\tilde{x} \in \mathcal{F}_k$ that satisfies $h(\tilde{x}) = \tilde{h}$, or $\tilde{f} = -\infty$ in the case where $\tilde{h} = h_{\max}$. It follows that

$\tilde{h} > h(p_k)$ and $\tilde{f} < f(p_k)$. Therefore, for sufficiently small $\Delta_k < \epsilon$, we have $h(p_k) < h(p_k + \Delta_k d) < \tilde{h}$ and $f(p_k) < f(p_k + \Delta_k d) < \tilde{f}$; thus, the trial mesh point is unfiltered, a contradiction. ■

A limitation of this result is that, while it prevents a non-stationary p_k from being a mesh-isolated poll center for infinitely many consecutive iterations, it does not completely prevent the algorithm from stalling there. The algorithm could still generate an infinite number of consecutive iterations in which p_k is either a mesh-isolated filter point or a filter point that does not generate a new poll center. If, for example, p_k simply alternates between these two possibilities, then Theorem 5.22 holds, but the algorithm still stalls at p_k .

As in previous results, the additional hypothesis of $p_k = p_k^F$ for infinitely many $k \in K$ would fully prevent stalling because it would force $h(p_k) = 0$ for infinitely many $k \in K$, and the strict differentiability of f at p_k means that $\nabla^c f(p_k)d < 0$ for some direction $d \in D_k(p_k)$. Thus, for sufficiently large $k \in K$, Δ_k is sufficiently small to force $f(p_k + \Delta_k d) < f(p_k)$, and the algorithm moves to a new point.

Remark 5.23 *Many of results in this and the previous subsections also apply to additional directions, which are specifically identified in [8]. We have not included this in our presentation because it would require an extraordinary amount of additional material to explain it properly. Since it is not possible to ensure convergence to a KKT point, the extra material adds little to the overall convergence theory. Instead, we refer the interested reader to [8] for a thorough discussion.*

6 Thermal Insulation System Design

We applied our algorithm to a problem in the design of a load-bearing thermal insulation system. The problem is fully described in [2] as an extension of the problem described in [20], in which we add realistic nonlinear constraints on stress, weight, and thermal contraction. In the next two subsections, we briefly describe the problem and provide some numerical results.

6.1 MVP Problem Formulation

Figure 4 (taken from [2]) shows a thermal insulation system of fixed length L with hot and cold surfaces having specified temperatures T_H and T_C , respectively. A certain number of shields or intercepts are inserted with insulators of various types and thicknesses between each pair of intercepts. The objective is to minimize the power f required to keep the intercepts at their temperatures. The decision variables for this problem are the number of intercepts n and their temperatures $T \in \mathbb{R}^n$, along with the insulator types $I \in \mathcal{I}^{n+1}$ and thicknesses $x \in \mathbb{R}^{n+1}$, where \mathcal{I} denotes the set of possible material types. Note that x and T are continuous variables, while n and I are categorical.

The cross-sectional areas A of the insulators are also variables (as indicated by the drawing in Figure 4), but in the process of adding nonlinear constraints on stress, weight, and thermal contraction, we can make a key observation (described in [2]) to combine the stress and weight constraints and eliminate A as a variable. Thus, we add a stress-weight constraint g_1 and a thermal contraction constraint g_2 , giving us the following optimization problem formulation:

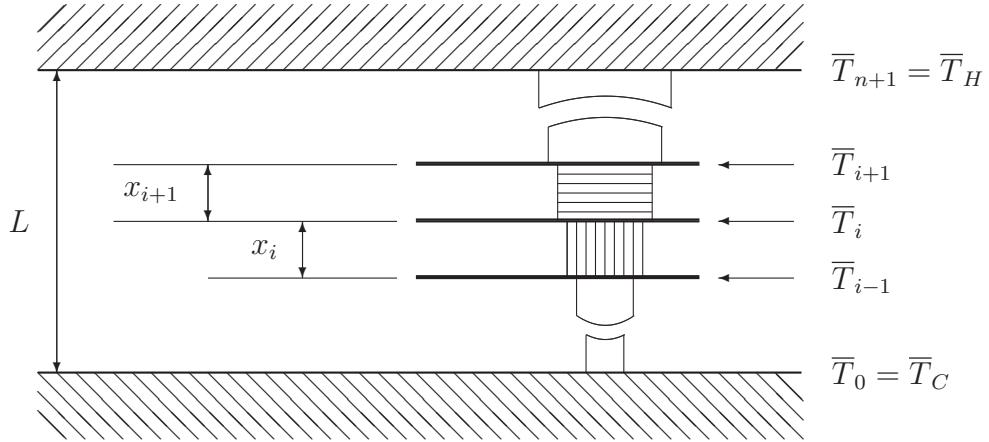


Figure 4: Schematic of a Thermal Insulation System (taken from [3])

$$\begin{aligned}
 & \min_{(n, I, x, T) \in X} f(n, I, x, T) \\
 \text{subject to } & g_1(n, I, x, T) \leq 0 \\
 & g_2(n, I, x, T) \leq 0 \\
 & n \in \mathbb{Z}^+ \\
 & I \in \mathcal{I}^{n+1} \\
 & \sum_{i=1}^n x_i \leq L \\
 & x_i \geq 0, \quad i = 1, \dots, n \\
 & T_{i-1} \leq T_i \leq T_{i+1}, \quad i = 1, \dots, n.
 \end{aligned} \tag{13}$$

A difficulty in solving this problem is that the dimension of the vectors I , x , and T depend on the variable n . For any value of n , there are $n + 1$ other categorical variables and $2n$ continuous variables, yielding a total of $3n + 2$ variables.

As in [20], we define local optimality in terms of the set of discrete neighbors \mathcal{N} obtained by

- changing the type of any one insulator;

- removing any one heat intercept and adjacent insulator;
- adding an intercept and insulator at any location.

6.2 Numerical Results

When applying Filter-MVPS to the problem described in Section 6.1, we achieved a 50% reduction in objective function value from that of the previous work of Hilal and Eyssa [18]. Our objective function value is very close to that of [20], in spite of the additional constraints, but the insulator configuration is quite different. The filter logic takes the algorithm to a different local minimizer.

To match the setup of [20] as much as possible, runs were performed with an initial mesh size of $\Delta_0 = 10$ and terminated when the condition $\Delta_k \leq .15625$ was achieved. An accelerated mesh refinement strategy was used, in which the mesh refinement exponent m_k^- (see (7)) was decremented at every mesh local optimizer. Coarsening of the mesh was not performed. The initial design consisted of one intercept placed exactly in the middle of the system and set at 150 K, with a nylon insulator on the cold side and a teflon insulator on the hot side.

No SEARCH step was used, and polling was performed about both the best feasible and least infeasible points. Extended poll triggers for the objective and constraint violation function were set at one and five percent, respectively, of the current objective function value, the former being consistent with [20]. Other initial data, including limits on stress, mass, and thermal contraction, are given in [2].

Figure 5 illustrates the performance of the FMVPS algorithm on the fully constrained model, where the power required for the incumbent best design is plotted versus the number of function evaluations. The lower plot is a magnification of upper one. The “L”-shaped plot is very typical behavior of derivative-free methods, since good stopping rules for these methods are difficult. The “stair steps” seen in the lower plot indicate varying length polling sequences.

Figure 6 depicts the progression of the filter during the run of the full model, where the plots in the right column are magnifications of those on the left. Each of the three rows represents a “snapshot” taken after 150, 300 respective function evaluations were performed. Although the algorithm terminated after more than 5500 function evaluations, changes in the filter after 300 function evaluations could not be detected within the resolution of the plot. This is consistent with the long and shallow progression of the best objective function value seen in Figure 5. Clearly, better stopping rules would be useful.

In the filter plots, the asterisks represent a subset of the best feasible points found up to that point, while the “stair step” lines represent the boundary between the filtered and unfiltered points. In this run, the nonlinear constraints were scaled by dividing each by its

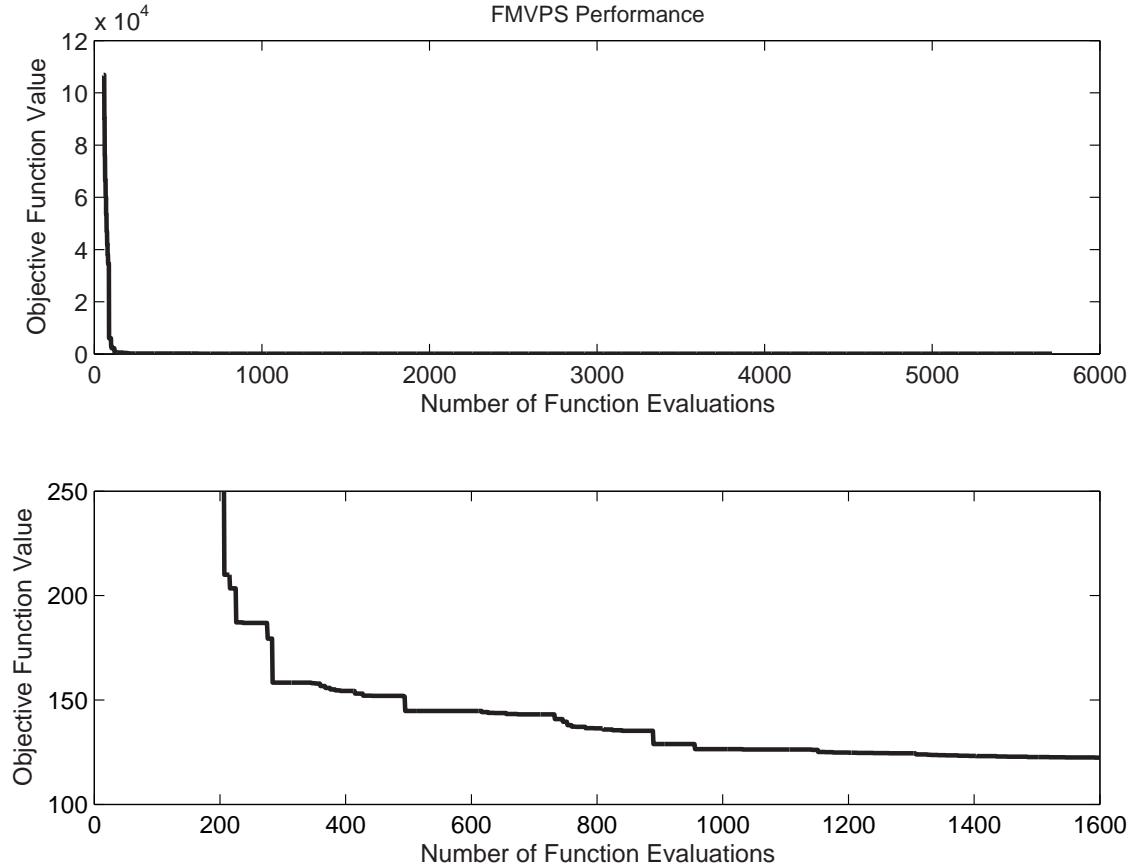


Figure 5: Iteration History for the Thermal Insulation System Design Problem

right-hand side and then subtracting one from both sides. Thus in the left column plots, the choice of $h_{\max} = 1$ represents a 100% constraint violation.

We should note that the objective function values shown on the vertical axes in both Figures 5 and 6 do not match those of [20] because they represent two different things. The objective function is to minimize power, as measured in both figures, but the required power shown in [20] is normalized with respect to system length and cross-sectional areas, so as to allow comparisons with the results of Hilal and Eyssa [18].

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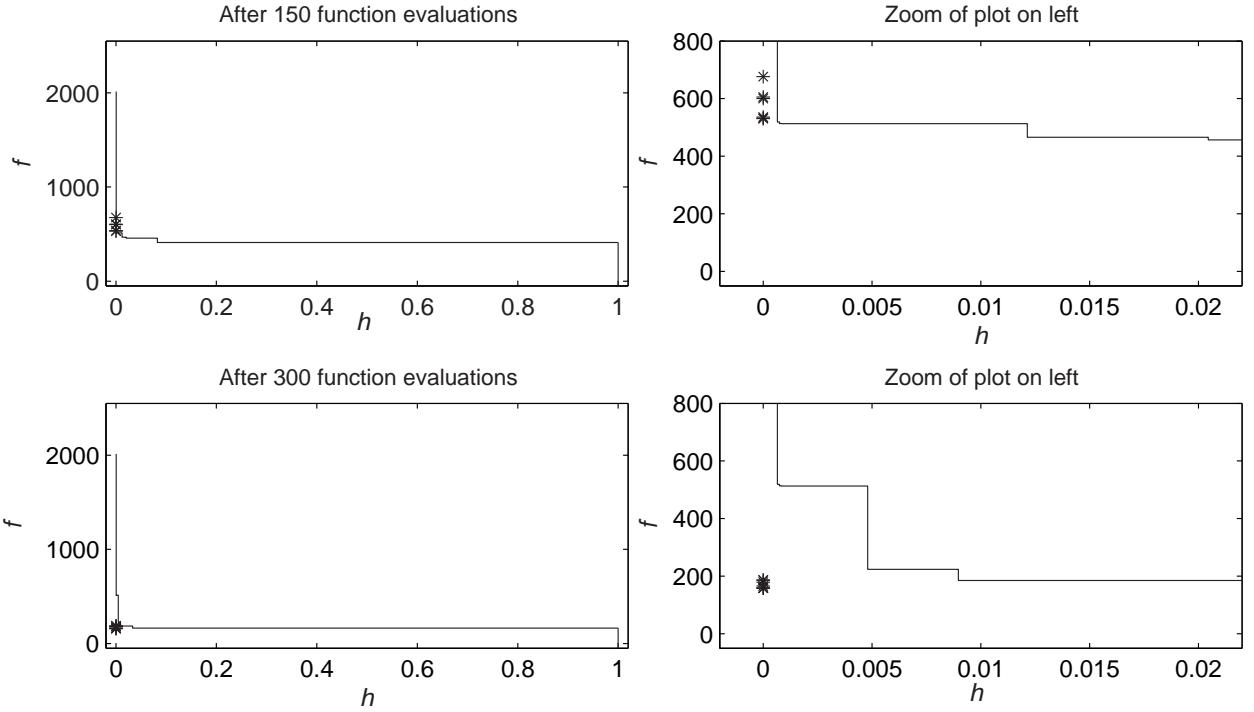


Figure 6: Filter Progression for the Full Model

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